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ABSTRACT

With an ever-increasing interest in water properties, many intermolecular force fields have been proposed to describe the behavior of water. Unfortunately, good models for liquid water usually cannot provide simultaneously an accurate melting point for ice. For this reason, the TIP4P/Ice model was developed for targeting the melting point and has become the preferred choice for simulating ice at coexistence. Unfortunately, available data for its dynamic properties in the liquid state are scarce. Therefore, we demonstrate a series of simulations aimed at the calculation of transport coefficients for the TIP4P/Ice model over a large range of thermodynamic conditions, ranging from $T = 245$ K to $T = 350$ K, for the temperature, and from $p = 0$ to $p = 500$ MPa, for the pressure. We have found that the self-diffusion (shear viscosity) exhibits smaller (increased) values than TIP4P/2005 and experiments. However, rescaling the temperature with respect to the triple point temperature, as in a corresponding states plot, we find that TIP4P/Ice compares very well with TIP4P/2005 and experiment. Such observations allow us to infer that despite the different original purposes of these two models examined here, one can benefit from a vast number of reports regarding the behavior of transport coefficients for the TIP4P/2005 model and utilize them following the routine described in this paper.

I. INTRODUCTION

Water is one of the most ubiquitous substances on earth. Hence, it is not surprising that great experimental and computational efforts have been devoted to investigate its properties. Such measurements are of great practical significance, but they have shown also that water exhibits a large number of interesting anomalies. These range from the well-known negative expansion coefficient below 4 °C, to the sharp increase of response functions such as compressibility upon cooling.[1]

This anomalous behavior also extends to the dynamic properties and transport coefficients. Since the end of the 19th century, it is known that viscosity of water decreases with the increase of pressure.[2] On the other hand, the diffusion coefficient increases as a function of pressure for both translation and rotation. This unusual behavior of transport properties is related to the breakage of the hydrogen bond network upon compression.[3] Indeed, the conversion between highly ordered tetrahedral water arrangements and disordered domains of high density are in the origin of most of water's anomalies.[4] This equilibrium, which persists in room temperature water, can be traced back to thermodynamic anomalies of metastable, supercooled water.[5] Therefore, the properties of supercooled water have been extensively studied, including the fragile-to-strong transition,[6,7] and the preservation of the Stokes–Einstein relation.[8,9]

The signature of bulk water's anomalies is also relevant to the study of interfaces. Particularly, the interface of supercooled liquid water in carbon nanotubes[10] and slit pores[11] exhibits giant slip lengths, which increase upon cooling and appear to be related with the failure of low-temperature bulk water to follow the Stokes–Einstein relation. Similarly, the understanding of surface premelting[12,13] and interfacial premelting,[14] as well as the related properties of the resulting quasi-liquid layer (QLL), has been the matter of intense debate.[15–17] For ice premelting, for example,

computer simulation studies show enhanced diffusivity of molecules at the water/vapor surface,[15,17,18] but intriguingly, some experiments claim a strong increase of viscosity of the premelting films relative to bulk values.[19,20]

In this regard, *in silico* studies of water properties provide very useful complementary information to experiments. Of course, such effort largely relies on the availability of intermolecular force fields, which are parameterized in such a way as to be able to reflect behavior of water as close as possible. Among the most popular point charge models, one can mention TIP4P[21] and its extended version TIP4P/2005;[22] SPC/E,[23] TIP5P,[24] and many others.[25] Unfortunately, it appears that point charge models, which are very good at predicting liquid water properties, cannot simultaneously provide an accurate melting point for ice.[26] In order to study the ice and ice–vapor equilibrium properties, which are of great importance for the determination of growth rates and shapes of snowflakes,[27] friction and lubrication of surfaces,[28] and many other important phenomena,[29] the TIP4P/Ice model has been developed.[30] This force field exhibits a melting temperature of $T \approx 270$ K[31] in ambient conditions, which is very close to the experimental result, and also reproduces the melting line. Therefore, it is pivotal to have a comprehensive outlook into the bulk water properties of the TIP4P/Ice model for studies of ice and water coexistence. However, it is worth emphasizing that, while it is easy to find values of transport coefficients for different water models in a variety of system conditions,[9,32,33] the literature data for TIP4P/Ice model has hardly been explored, except for a limited number of thermodynamic states.[15,17,34–36]

In view of this, the aim of this paper is to calculate both diffusion coefficients and shear viscosities of the TIP4P/Ice model over a large range of thermodynamic conditions, from ambient temperature to the undercooled regime, as well as for a large range of pressures, spanning atmospheric conditions to the hundreds of MPa.

II. METHODS

To determine the diffusion coefficient, we have used the Einstein relation, which involves the calculation of mean squared displacement (MSD) of individual water molecules:

$$\left\langle \Delta r^2(t) \right\rangle = \left\langle (\mathbf{r}(t) - \mathbf{r}(0))^2 \right\rangle, \tag{1}$$

where $\mathbf{r}(t)$ is the position of a water molecule at time t, and the triangular brackets denote a thermal average over all time origins and individual particles. For an n-dimensional system, the MSD is linear with time, and the slope is related to the diffusion coefficient D as $\left\langle r^2(t) \right\rangle = 2nDt$.[37]

In order to calculate the viscosity, we have employed the Green–Kubo relation, which involves the calculation of autocorrelation functions of components of the stress tensor as

$$G_{\alpha\beta} = \frac{V}{k_B T} \left\langle \sigma_{\alpha\beta}(t) \sigma_{\alpha\beta}(0) \right\rangle, \tag{2}$$

where V is the volume of the system, $\sigma_{\alpha\beta}$ represents the $\alpha, \beta = x, y, z$ component of the stress tensor, and k_B is the Boltzmann constant.[37]

To improve the statistics, we do not restrict to the off-diagonal components of the stress tensor. Daivis and Evans have shown that the diagonal components of the stress tensor are larger by the factor of $2 - (2/n)$ than the off-diagonal elements, where n is the dimensionality of the system.[38] Therefore, one can use all of the six components of the stress tensor in the calculation of the shear viscosity, just given the fact that they are scaled by the adequate factor. Knowing that, the shear viscosity is then calculated as

$$\eta = \int_0^\infty G_\eta(t) dt, \tag{3}$$

where $G_\eta(t) = \frac{1}{6}[G_{xy} + G_{xz} + G_{yz} + \frac{3}{4}(G_{xx} + G_{yy} + G_{zz})]$.

Water was modeled with the use of the TIP4P/Ice force field.[30] The number of water molecules was equal to 1280 for all systems studied. We decided to use such system size to avoid system size effects due to insufficient number of molecules and yet being able to perform simulations in a reasonable time, which is particularly important in the case of the shear viscosity, as these calculations are computationally expensive. Molecular dynamics simulations of bulk water were performed using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) package.[39] Trajectories were evolved using the velocity Verlet algorithm, with a 2 fs time step. Bonds and bond angles were constrained by the use of the SHAKE algorithm. Both the temperature and pressure were set using Nose–Hoover chain algorithms,[40,41] with damping factor $\tau = 2$ ps and the number of chains $M = 3$. To remain consistent with the definition of TIP4P/Ice, all dispersion interactions were truncated at 8.5 Å. Long-range Coulombic interactions were computed using the particle–particle particle-mesh method.[42] The charge structure factors were evaluated with the fourth-order interpolation scheme and a grid spacing of 1 Å, resulting in 36, 32, and 36 vectors in the x, y, and z directions in reciprocal space, respectively.

The simulation scheme involved two steps. In the first one, simulations for bulk water have been performed for 15 ns in the NpT ensemble, in order to obtain an accurate average density. Then, the system was accordingly rescaled to the given average density, and further 40 ns runs in the NVT ensemble were performed, in which the relevant trajectories for the calculation of transport coefficients have been gathered over the last 30 ns, every 15 ps. For the calculation of shear viscosities, the stress tensor components have been printed every 10 fs. Although the pressure in the NVT ensemble will not be exactly the one input in NpT simulations, the uncertainty in the precise value is marginal. Such a two-step simulation scheme is also common practice for the estimation of the lateral area necessary for the calculation of solid–liquid coexistence curves by the use of direct coexistence method.[43,44] However, to avoid confusion, Table I presents both the input pressure and density used during NpT and NVT simulations, respectively. Simultaneous evaluation of the diffusion coefficients and shear viscosity has a particular advantage, in that one can test their coupling right away using a single molecular dynamics simulation. Moreover, calculation of transport properties in the NVT ensemble does not perturb the dynamics of the pressure tensor, which could influence the obtained values of shear viscosities. On top of that, based on the systematic study of Basconi and Shirts,[45] reporting the impact of different thermostats

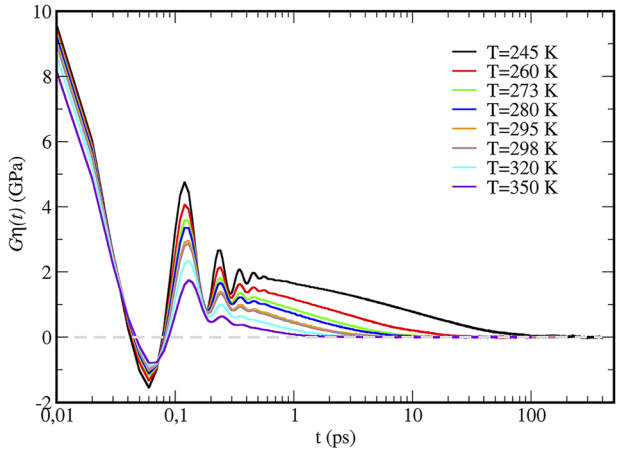

FIG. 1. Stress autocorrelation functions $G_\eta(t)$ evaluated at different temperatures in ambient pressure, p = 0 MPa.

and their coupling strength, such simulation scheme should lead to the most reliable results.

Following the above simulation scheme, the translational mean square displacement and shear viscosities were calculated at eight different temperatures, spanning from T = 245 K to T = 350 K, in the pressure range p = 0–500 MPa. In all the conditions studied, the linear regime of MSD has been established, starting from the first saved configuration. However, in the case of the Green–Kubo autocorrelation functions, the numerical integration by trapezoidal rule had to be performed up to the upper limit, denoted as τ_α. Its value has been estimated by the inspection of a characteristic timescale where the autocorrelation function smoothly decays to 0, so that the contributions from the long tail to the integral, which are subject to the random noise, are omitted. Averaged Green–Kubo autocorrelation functions, evaluated at different temperatures at ambient pressure can be found in Fig. 1. One can see that there is a significant change in the characteristic timescale τ_α, which increases upon cooling and reaches up to 200 ps for the lowest temperature (cf. Table I in Appendix).

III. RESULTS

The isotherms for a given transport coefficient examined in the paper are presented in Fig. 2 and can also be found in Table I shown in Appendix. Let us now compare currently obtained results with the available experimental data. For instance, at ambient pressure, with this model we obtain $D = 12.368 \times 10^{-10}(\mathrm{m^2\ s^{-1}})$ and $D = 5.079 \times 10^{-10}(\mathrm{m^2\ s^{-1}})$, compared to experimental values of $D_{\mathrm{exp}} = 23 \times 10^{-10}(\mathrm{m^2\ s^{-1}})$[46] and $D_{\mathrm{exp}} = 10.9 \times 10^{-10}(\mathrm{m^2\ s^{-1}})$[47] at T = 298 K and T = 273 K, respectively. One can see that the values of the self-diffusion coefficients are lower than those reported experimentally. On the other hand, the viscosities of liquid water are higher than experimental values,[48] which is not surprising, due to the Stokes–Einstein relation. Consequently, the aforementioned observations concern all other points studied. It is worth highlighting

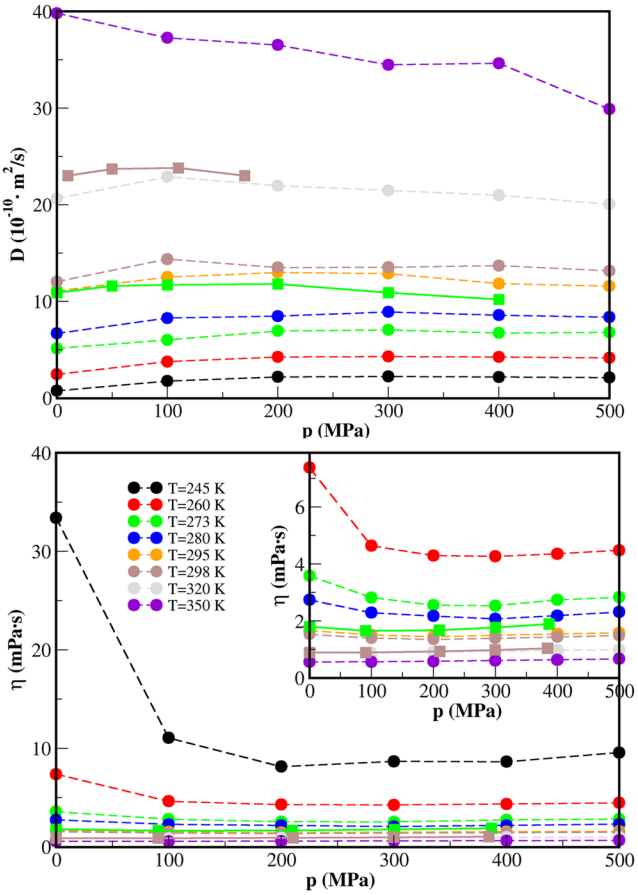

FIG. 2. Relation of self-diffusion coefficient (top) and viscosity (bottom) with respect to pressure. Circles (dashed line) and squares (solid lines) represent TIP4P/Ice and experimental values, respectively. Labels are the same for both panels. Inset to the bottom part displays the magnified data.

that the decreased (increased) value of diffusion coefficient (shear viscosity) has already been noted and is consistent with other papers.[15,25]

In view of this fact, it is well-known that TIP4P/2005 is widely used due to its successful description of liquid water properties, consistent with experimental data. Therefore, it seems reasonable to validate our current simulation results with those obtained for TIP4P/2005 model. Figure 3 shows a comparison between our simulations and those performed by Montero de Hijes *et al.*[33] Indeed, one can see the same behavior for the transport coefficients, that, as stated before, TIP4P/Ice exhibits a decreased (increased) value of diffusion coefficient (shear viscosity) compared to TIP4P/2005 water model in the whole range of points studied. We conjecture that this behavior can be congruent with the shift in the melting point (T_m) of ice Ih and triple points (T_t) of these models. They were reported to be as $T_{2005,m} \approx 250$ K[31] and $T_{2005,t} = 252.1$ K,[49] and $T_{ice,m} \approx 270$ K[31] and $T_{ice,t} = 272.2$ K,[49] for TIP4P/2005 and TIP4P/Ice, respectively.

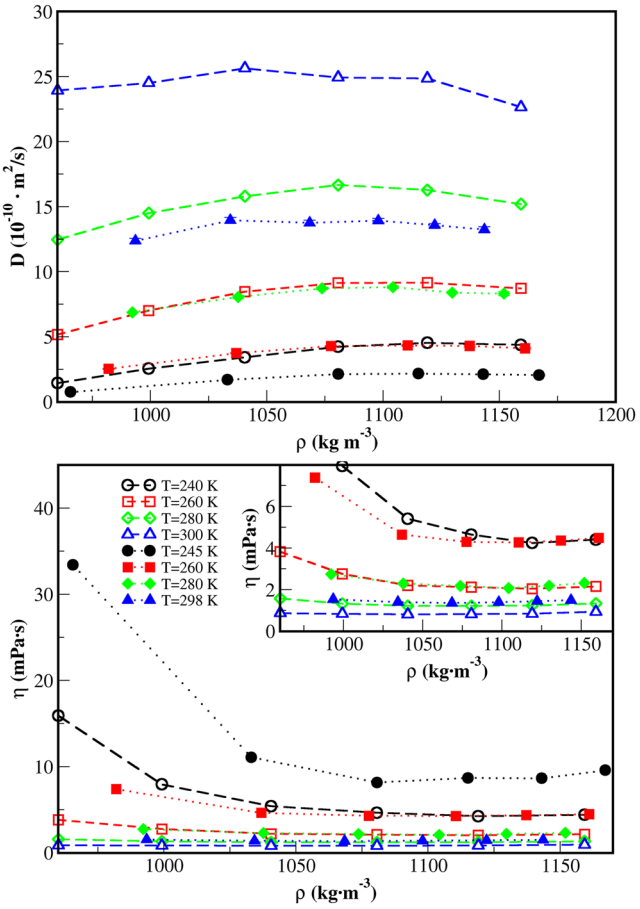

FIG. 3. Relation of self-diffusion coefficient (top) and viscosity (bottom) with respect to density. Filled and open symbols depict currently obtained data for TIP4P/Ice and TIP4P/2005 from Ref. 33, respectively. Labels are the same for both panels. Inset to the bottom part displays the magnified data.

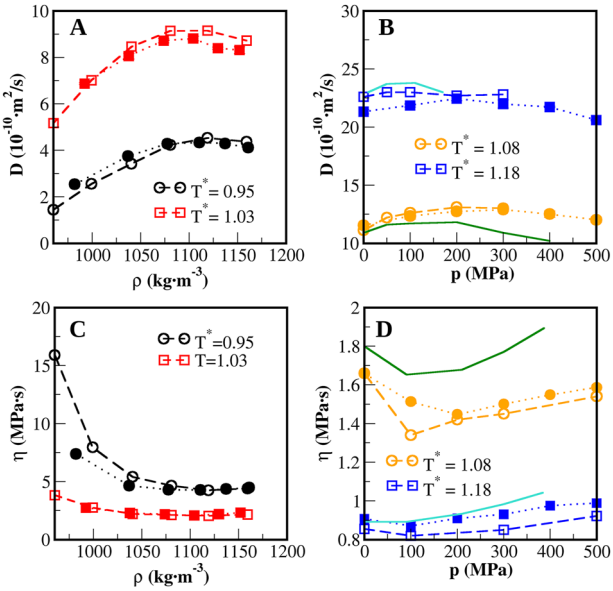

FIG. 4. Relation of self-diffusion coefficient (a) and (b), and viscosity (c) and (d), with respect to density or pressure. Filled and open symbols depict currently obtained data for TIP4P/Ice and TIP4P/2005 from Ref. 33 [parts (a) and (c)] and Ref. 32 [parts (b) and (d)], respectively. Solid lines correspond to the experimental data taken from Refs. 46–48.

Therefore, a naturally arising question is whether the origin of these differences is just due to the temperature shifts, or, as the models were parameterized to describe different features of water, exhibiting different transport properties is a natural consequence. Here, we aim to answer these questions. In order to do that, we assumed that the simulation points for different models should be presented in reduced units. We mapped the points by the law of corresponding states, reduced by the triple points of TIP4P/2005 and TIP4P/Ice models, i.e., $T^* = T_X/T_{X,t}$, where X is either TIP4P/2005 or TIP4P/Ice. It has to be emphasized that the ratio T_m/T_c between melting and critical points of the TIP4P2005 and TIP4P/Ice models is equal to 0.39 and 0.383, respectively (see Table V of Ref. 49 for critical point estimation). In other words, there is no significant difference as to whether we choose to rescale the temperature by a triple point or critical point (aside from the temperature scale) to preserve the universal features shown later on. The results can be found in Fig. 4 and Tables II and III in Appendix.

One can now see an excellent agreement between the two models when expressed in reduced units. Such observation refers both to the self-diffusion and shear viscosities. Although one can easily notice that there is a mismatch in the comparison between current simulation results and the points extracted from Montero de Hijes *et al.*[33] [Figures 4(a) and 4(c)], the trends are still preserved within the whole range of points studied. Differences in the examined densities result from the different approaches in our and their paper. In other words, we wanted to examine the behavior in a wide pressure range for TIP4P/Ice model, rather than explicitly match points from other papers. Nevertheless, we can observe nearly perfect agreement between two models and also with experimental data. It has to be noted that, while for viscosity, it seems that the differences are quite large, they, in fact, differ by just about 10%, however, still preserving the trend observed experimentally. It now seems to be clear that the answer to the origin of the differences in transport coefficients of TIP4P/2005 and TIP4P/Ice models can be attributed to the different absolute temperature scales. In practice, for comparison with experiments, this means that transport properties obtained at temperature T from the TIP4P/Ice model are good estimates of liquid water properties at an effective temperature of $T_{ef} = \frac{T_{t,2005}}{T_{t,Ice}} T$.

According to the Stokes–Einstein relation, the self-diffusion of a spherical particle can be related to the viscosity of the surrounding media as $D = k_B T/3\pi\eta a$, where a is the molecular diameter. Surprisingly, there exists ample evidence that this hydrodynamic result also holds quite accurately down to molecular scales. Analogous to other water models and experimental systems, we checked

the Stokes–Einstein (SE) relation for the TIP4P/Ice model, by plotting $D\eta/T$ as a function of temperature. The results are presented in Fig. 5. To show the temperature variation of $D\eta/T$, it has been normalized by the reference temperature, which usually is the highest temperature examined. In our case, it is taken to be $T = 350$ K at all pressures studied. We can see that at pressures higher than $p = 200$ MPa, the deviations start to occur already at $T = 320$ K, and at a somewhat lower temperature of $T = 298$ K, for all the remaining pressures. This is consistent with previous work reporting the violation of the SE relation for temperatures way higher than those in regular supercooled liquids, which usually is $1.3T_g$, where T_g is the vitrification temperature (for water $T_g \approx 136$ K). On the other hand, it has to be noted that, aside from the lowest temperature studied, $T = 245$ K, the deviation is still moderate and does not exceed 30%. Importantly, the deviations are roughly independent on the pressure. Therefore, the SE relation does not serve as a quantitative theory, but it is still useful as an order of magnitude estimate of the viscosity for the TIP4P/Ice model down to $T = 245$ K, given that one can obtain values of viscosity from the self-diffusion coefficients using the Stokes–Einstein relation $\eta = \frac{k_B T}{3\pi D a}$, within an acceptable error margin, with $a \approx 2.8$ Å being the position of the first maximum in the radial distribution function r_{OO} between oxygens in water. The introduction of such definition, rather than the molecular diameter of water, is motivated by the fact that its tetrahedral structure is mainly dominated by the presence of hydrogen bonds.

Since the SE relation is violated, having calculated the values of self-diffusion coefficient and shear viscosity for a series of isotherms, it is also interesting to check what is this hydrodynamic diameter ϕ_h that is required to obey the SE relation exactly. It can be extracted as follows:

$$\phi_h = \frac{k_B T}{3\pi\eta D}. \tag{4}$$

Figure 6 shows ϕ_h calculated from the simulation data. Compared to the position of the first maximum in the radial distribution function

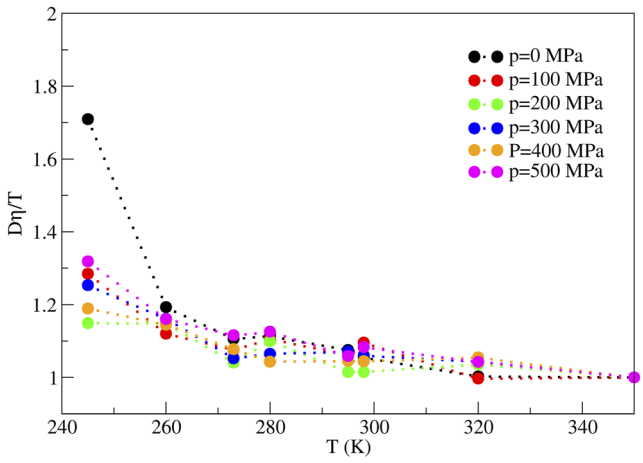

FIG. 5. Relation of $D\eta/T$ with temperature, normalized at $T = 350$ K, for all pressures studied.

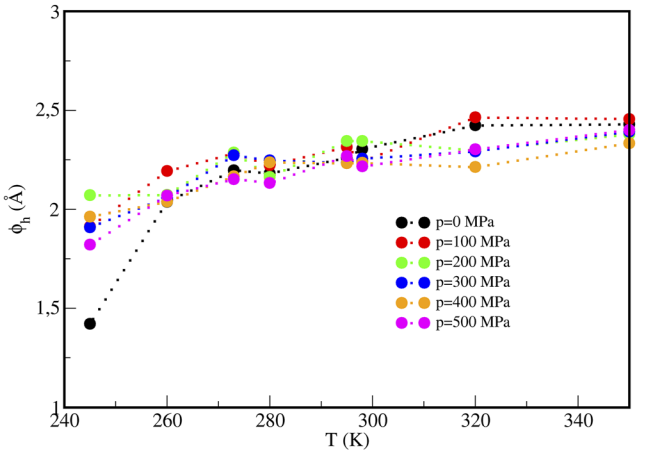

FIG. 6. Temperature dependence of hydrodynamic diameter ϕ_h for all pressures studied.

$r_{OO} \approx 2.8$ Å, it exhibits a smaller value at all temperatures studied. ϕ_h is independent of the pressure and decreases with temperature; however, the deviations from r_{OO} do not exceed 30%, except for the outlier at $T = 245$ K at ambient pressure. This feature of decreasing ϕ_h upon cooling has been observed in many fragile glassformers.[50]

IV. CONCLUSIONS

In this paper we computed the transport coefficient of bulk liquid water, using TIP4P/Ice model at eight different temperatures, ranging from $T = 245$ K to $T = 350$ K, in a pressure range $p = 0$–500 MPa. We emphasize that, to our knowledge, such a systematic study for this particular water model has not been performed to date. We have shown that the self-diffusion (shear viscosity) exhibits decreased (increased) values than experimental findings or those extracted from the TIP4P/2005 water model. However, if one would switch to the reduced units formalism, with respect to the model's triple point (or critical point), the behavior changes dramatically. In such a case, models are now in excellent agreement with each other and also reflect experimental data nearly quantitatively. Such observations allow us to infer that despite different original purposes of models considered here, one can benefit from a vast number of reports regarding the behavior of transport coefficients for TIP4P/2005 model and utilize them following the routine described in this paper. It seems that the answer to the origin of the differences in transport coefficients between models is merely because of different absolute temperature scales.

Despite that, we would like to emphasize that we did not study deeply the supercooled regime and, therefore, cannot guarantee that this is a universal feature, so, a special caution has to be paid. Moreover, in view of these findings, the naturally arising questions are: Is the behavior the same as regards other quantities, such as the dielectric constant,[51] surface tension,[52] densities of ices, and perhaps other[53]? Is this the universal feature for all water models? Our results suggest that the analogy could be exploited at least for the study of transport properties, so that accurate data for a model with unknown

transport coefficients could be inferred from other models with known transport properties.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Łukasz Baran: Formal analysis (equal); Investigation (lead); Writing – original draft (lead). **Wojciech Rżysko**: Formal analysis (equal). **Luis G. MacDowell**: Conceptualization (lead); Writing – original draft (supporting).

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

APPENDIX: SIMULATION DATA

All of the simulation points are presented in Table I, with the uncertainties presented in the form of standard errors. The calculation of uncertainties for the viscosity was straightforward, as we obtained six independent integrals of autocorrelation functions of the traceless stress tensor elements. In the case of self-diffusion coefficients, we have followed the same routine as in the Ref. 33 Briefly, the trajectory was divided into four blocks of same duration, equal to 7.5 ns, and for each of them, the self-diffusion coefficient was calculated as the slope of the mean-squared displacement, as explained in Sec. II.

TABLE I. Simulation results of TIP4P/Ice water model for the shear viscosity and diffusion coefficients. τ_α depicts the upper limit in the integral over the autocorrelation functions. The standard errors are given in parentheses.

T (K)	p (MPa)	ρ (kg m^{-3})	D (10^{-10} m^2 s^{-1})	η (mPa s)	τ_α (ps)
245	0	965.62	0.756 (0.013)	33.392 (2.890)	200
	100	1033.12	1.696 (0.020)	11.069 (0.186)	50
	200	1080.76	2.126 (0.016)	8.151 (0.17)	30
	300	1115.19	2.166 (0.019)	8.681 (0.224)	35
	400	1143.04	2.117 (0.022)	8.641 (0.149)	37.5
	500	1167.10	2.058 (0.063)	9.578 (0.192)	50
260	0	982.01	2.533 (0.032)	7.379 (0.197)	55
	100	1036.89	3.744 (0.041)	4.638 (0.084)	30
	200	1077.63	4.283 (0.036)	4.291 (0.137)	27.5
	300	1110.59	4.334 (0.064)	4.265 (0.083)	25
	400	1137.21	4.291 (0.089)	4.355 (0.098)	20
	500	1161.02	4.110 (0.050)	4.479 (0.070)	17.5
273	0	989.63	5.079 (0.096)	3.585 (0.076)	20
	100	1037.72	6.212 (0.030)	2.821 (0.0604)	20
	200	1075.34	6.845 (0.039)	2.555 (0.044)	10
	300	1106.45	6.946 (0.063)	2.533 (0.019)	10
	400	1132.31	6.742 (0.060)	2.739 (0.033)	10
	500	1155.31	6.561 (0.036)	2.832 (0.035)	10
280	0	992.24	6.866 (0.040)	2.738 (0.069)	15
	100	1037.71	8.054 (0.125)	2.292 (0.011)	15
	200	1073.73	8.717 (0.095)	2.175 (0.031)	15
	300	1104.23	8.810 (0.102)	2.072 (0.029)	10
	400	1129.72	8.392 (0.049)	2.185 (0.017)	10
	500	1151.99	8.312 (0.148)	2.313 (0.013)	10
295	0	993.95	11.528 (0.231)	1.658 (0.008)	10
	100	1035.53	12.341 (0.283)	1.513 (0.011)	8
	200	1069.76	12.734 (0.169)	1.447 (0.016)	7
	300	1098.51	12.892 (0.027)	1.500 (0.014)	7
	400	1123.58	12.501 (0.283)	1.549 (0.022)	6
	500	1145.33	12.009 (0.043)	1.586 (0.014)	7
298	0	993.51	12.368 (0.198)	1.532 (0.024)	8
	100	1034.35	13.949 (0.228)	1.396 (0.011)	8
	200	1068.45	13.752 (0.207)	1.354 (0.017)	7
	300	1097.94	13.922 (0.162)	1.390 (0.019)	7
	400	1122.17	13.564 (0.126)	1.441 (0.013)	6
	500	1143.57	13.236 (0.219)	1.488 (0.014)	7
320	0	990.33	21.317 (0.194)	0.907 (0.011)	5
	100	1028.62	21.856 (0.132)	0.870 (0.009)	4
	200	1061.28	22.447 (0.191)	0.909 (0.004)	4
	300	1089.26	21.983 (0.350)	0.930 (0.007)	4
	400	1113.14	21.723 (0.059)	0.975 (0.012)	4
	500	1134.37	20.598 (0.069)	0.988 (0.008)	3
350	0	979.43	37.512 (1.116)	0.562 (0.006)	4
	100	1017.62	36.706 (0.250)	0.569 (0.005)	2.5
	200	1049.17	36.923 (0.426)	0.584 (0.001)	2.5
	300	1075.84	34.953 (0.279)	0.613 (0.002)	2.5
	400	1099.59	34.474 (0.232)	0.637 (0.004)	2
	500	1120.75	31.801 (0.303)	0.672 (0.003)	2

Tables II and III show the comparison of the transport properties of liquid water of TIP4P/2005 and TIP4P/Ice water models at the reduced temperatures. As described in the text, there is an excellent agreement between the models, as well as with experimental findings.

TABLE II. Comparison of simulation results for two water models for the self-diffusion coefficient D at 10^{-10} m^2 s^{-1}. Experimental temperature is the same as for TIP4P/2005. Experimental values are taken from Refs. 46 and 47, whereas for TIP4P/2005, they are extracted from Ref. 54.

T^*	$p_{\mathrm{TIP4P/2005}}$	$p_{\mathrm{TIP4P/Ice}}$	$p_{\mathrm{expt.}}$	$T_{\mathrm{TIP4P/2005}}$	$T_{\mathrm{TIP4P/Ice}}$	$D_{\mathrm{TIP4P/2005}}$	$D_{\mathrm{TIP4P/Ice}}$	$D_{\mathrm{expt.}}$
1.08	0.1	0	0.1	273	295	11.1	11.53	10.9
	100	100	100	273	295	12.61	12.34	11.7
	200	200	200	273	295	13.1	12.73	11.8
	300	300	300	273	295	13	12.89	10.9
1.18	0.1	0	10	298	320	22.60	21.32	23.0
	100	100	110	298	320	23	21.86	23.8
	200	200	170	298	320	22.7	22.45	23
	300	300		298	320	22.8	21.98	

TABLE III. Comparison of simulation results for two water models for the shear-viscosity η in mPa·s. Experimental temperature is the same as for TIP4P/2005. Experimental values are taken from Ref. 48, whereas simulation points for TIP4P/2005 are taken from Refs. 54 and 32.

T^*	$p_{\mathrm{TIP4P/2005}}$	$p_{\mathrm{TIP4P/Ice}}$	$p_{\mathrm{expt.}}$	$T_{\mathrm{TIP4P/2005}}$	$T_{\mathrm{TIP4P/Ice}}$	$\eta_{\mathrm{TIP4P/2005}}$	$\eta_{\mathrm{TIP4P/Ice}}$	$\eta_{\mathrm{expt.}}$
1.08	0	0	0.1	273	295	1.66	1.66	1.799
	100	100	90.7	273	295	1.34	1.51	1.653
	200	200	209.6	273	295	1.42	1.45	1.678
	300	300	300.4	273	295	1.45	1.50	1.771
	500	500		273	295	1.54	1.59	
1.18	0	0	0.1	298	320	0.855	0.907	0.892
	100	100	90.7	298	320	0.819	0.870	0.891
	200	200	209.6	298	320	0.830	0.909	0.933
	300	300	300.4	298	320	0.85	0.930	0.983
	500	500		298	320	0.922	0.988	

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